Kondo Quantum Dots and the Novel Kondo-doublet interaction.

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We analyze the interactions between two Kondo Quantum Dots connected to a Rashba-active Quantum Wire. We find that the Kondo-doublet interaction, at an inter-dot distance of the order of the wire Fermi length, is over an order of magnitude greater than the RKKY interaction. The effects induced on the Kondo-doublet interaction by the wire spin-orbit coupling can be used to control the Quantum Dots spin-spin correlation. These results imply that the widely used assumption that the RKKY is the dominant interaction between Anderson impurities must be revised.

Introduction. Kondo Quantum Dots made in semiconductor heterostructures sparked a growing experimental and theoretical research in the area [1, 2, 3]. In those systems a correlated electronic state localized in a quantum dot (QD) interacts with a low dimensional electron gas via an hybridization term. They belong to the very rich family of physical systems that are described by the Anderson-Impurity Hamiltonian [4]. The Kondo Quantum Dots regime, in which a single electron is allowed in the QD top most populated orbital due to the Coulomb blockade effect, has attracted considerable interest due to the possibility of using the QD spin as a quantum bit [5, 6]. These systems have a relatively high Kondo ($\delta_K \simeq 1K$) to Fermi (E_F) energy ratio, corresponding to a strong Kondo coupling of the dot-band system [7]. The two Kondo QD problem is crucial for understanding how QDs interact, and how these interactions can be controlled. This has been the subject of several recent letters [8, 9, 10, 11, 12].

A common denominator of those letters is that they assume that the correlation between the QD's is given by the RKKY interaction [4, 13]. In the Kondo regime the RKKY is the strongest of the different fourth order interactions present in the two-QD Anderson Hamiltonian [14, 15, 16]. But it was recently found in Ref.[17] that the dominant interaction in the Kondo regime is the non-perturbative second order Kondo-doublet process.

The Kondo-doublet owes its strong Kondo-like correlation energy to the resonance of one of the sets of configurations that form its screening cloud. The set with one spin up electron in each QD plus a spin down hole in the band interact via the annihilation of the hole in any of the two QDs. Thus, the "connectivity" of this set is enhanced by the interference of these two paths. As the enhanced set is one of parallel QD-spins, the Kondo-doublet generates a strong ferromagnetic correlation between the QDs.

Therefore, two Kondo QDs connected to a Rashba active quantum wire (QW) is an ideal system to check the predictions of Ref.[17]. QDs-QW systems are experimentally accessible [7, 18]. A simple tool for fine tuning the interactions between the QDs is a tunable Rashba [19] spin-orbit coupling (RSO) of the band states [20], that makes the spin of the band excitations to precess. Such a system is also very important for the development of nanoscopic quantum electronics [5]. In the following we analyze the effects of the RSO interaction on the Kondo-doublet for a two-QD-QW setup. We compare our results with that of Imamura *et al* [21] for the RKKY interaction. We find that the Kondo-doublet interaction is over an order of magnitude greater than the RKKY interaction.

Model. For a quantum wire with RSO it is convenient to choose the spin quantification axis perpendicular to both the wire and the effective RSO electric field, conserving S_z as a good quantum number. Thus, with the wire along the x-axis and the RSO electric field applied in the y-axis the Hamiltonian for the conduction electrons is given by $H_b = -\frac{\hbar^2}{2m} \partial_x^2 - i \alpha \partial_x \sigma_z$, where α is the variable RSO coupling and σ_z the Pauli matrix. The spin-degeneracy of the band states is removed. The spin-up (down) k-states energy is now $e_{k\uparrow(\downarrow)} = \frac{\hbar^2}{2m}(k \pm k_s)^2 - \Delta_s$, where $k_s = \frac{m}{\hbar^2}\alpha$. The effect of the last term ($\Delta_s = \frac{\hbar^2}{2m} k_s^2$) is to lower the bottom of the band, increasing the electron density in the wire if the chemical potential is maintained fixed. In the following we disregard this term, working at fixed QW electron density, Fig. 1. If necessary, the effects of this term can be included in the final results by renormalizing the Fermi energy and wave-vector ($E_F \mapsto E_F + \Delta_s$ and $k_F \mapsto \sqrt{k_F^2 + k_s^2}$) [21]. We concentrate our work in the phase effects generated by the RSO.

The two-QD-QW Anderson Hamiltonian is the sum of the band, hybridization (H_V), and correlated QDs (with the QDs at $R_j = \pm R/2$) Hamiltonians

$$
H = \sum_{k\sigma} e_{k\sigma} c_{k\sigma}^\dagger c_{k\sigma} + \mathbf{v} \sum_{jk\sigma}(e^{i kR_j} d_{j\sigma}^\dagger c_{k\sigma} + h.c.)
$$
$$
- E_d \sum_{j\sigma} d_{j\sigma}^\dagger d_{j\sigma} + U \sum_j d_{j\uparrow}^\dagger d_{j\uparrow} d_{j\downarrow}^\dagger d_{j\downarrow} , \tag{1}
$$

where the fermion operator $c_{k\sigma}(d_{j\sigma})$ act on the conduc-

tion band k-state (on the QD at R_j) and $\mathbf{v} = V/\sqrt{L}$ is the hybridization divided by the square root of the wire length. We renormalize the vacuum (denoted by $|F\rangle$) to be the conduction band filled up to the Fermi energy and we make an electron-hole transformation for band states below the Fermi level: $b^\dagger_{k\overline{\sigma}} \equiv c_{k\sigma}$. Single state energies are referred to the Fermi energy. In the Kondo limit, the case analyzed in this work, the QD level is well below the Fermi energy ($-E_d \ll 0$), and it can not be doubly occupied due to the strong Coulomb repulsion ($U \gg E_d$). In this regime the two relevant Hamiltonian parameters are the effective Kondo coupling $J_n = \rho_o V^2/E_d$ (ρ_o being the density of band states at the Fermi level) and the inter-dot distance R. The single QD Kondo energy is given by $\delta_K = E_F \exp(-1/2J_n)$. We use in the text a "ket" notation for the QDs-band configurations, the first symbol indicates the status of the left QD (the one at $x = -R/2$) and the second one the status of the QD on the right, e.g. $|00\rangle \equiv |F\rangle$, $|0\uparrow\rangle \equiv d^\dagger_{R\uparrow}|F\rangle$, $|\downarrow\uparrow\rangle \equiv d^\dagger_{L\downarrow}d^\dagger_{R\uparrow}|F\rangle$, $|\downarrow\uparrow, h_{k\sigma}\rangle \equiv b^\dagger_{k\sigma}d^\dagger_{L\downarrow}d^\dagger_{R\uparrow}|F\rangle$, etc..
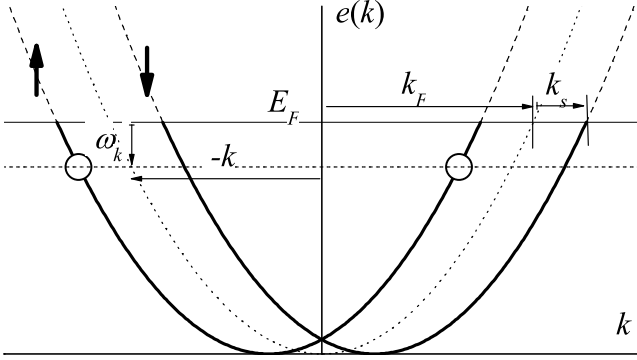

FIG. 1: Quantum wire energy bands. The spin-degeneracy is removed by the Rashba spin-orbit coupling. The circles on the spin up band mark the two spin down holes of energy w_k.

With the chosen axis the non-resonant set (composed by the $|\uparrow\downarrow, h_{k\uparrow}\rangle$ and $|\downarrow\uparrow, h_{k\uparrow}\rangle$ configurations) remains so due to S_z conservation. The effects of the RSO appear in the resonant set-vertex states connections (matrix elements). Due to the mirror symmetry breaking produced by the RSO the even and odd doublets are mixed. To trace these effects we select two components of the set, the ones with a hole of energy w_k. They correspond to the removal of the $k_- = -k - k_s$ ($|\uparrow\uparrow, h_{k_-\downarrow}\rangle$) or the $k_+ = k - k_s$ ($|\uparrow\uparrow, h_{k_+\downarrow}\rangle$) electron from the spin-up band, see Fig. 1. Applying H_V to the vertex state ($|A_\uparrow\rangle = |0\uparrow\rangle - |\uparrow 0\rangle$) of the odd doublet the following combination is generated

$$-(e^{i\varphi_+}+e^{-i\varphi_+})|\uparrow\uparrow, h_{k_+\downarrow}\rangle-(e^{i\varphi_-}+e^{-i\varphi_-})|\uparrow\uparrow, h_{k_-\downarrow}\rangle , \quad (2)$$

where $\varphi_\pm = k_\pm R/2$. The contribution of these configurations to the set connectivity is obtained by closing the

Kondo-doublet path (in units of $4V^2/L$),

$$\langle A_\uparrow|H_V^2|A_\uparrow\rangle_{\uparrow\uparrow} = 1 + \cos(kR)\cos(k_sR) , \quad (3)$$

the first term on the r.h.s. (1) comes from the hole being annihilated at the same QD where it was generated and the second term corresponds to the annihilation of the hole at the other QD. This last term includes the additional phase factor generated by the RSO. But now, due to the RSO symmetry breaking the configuration of (Eq.(2)) is also connected with the even doublet vertex state ($|S_\uparrow\rangle = |0\uparrow\rangle + |\uparrow 0\rangle$), given that

$$\langle S_\uparrow|H_V^2|A_\uparrow\rangle_{\uparrow\uparrow} = -i\,\cos(kR)\sin(k_sR) . \quad (4)$$

A straightforward analysis shows that the proper vertex states when the RSO is active is the twisted "odd" vertex

$$|\widetilde{A_\uparrow}\rangle = \cos\varphi_s|A_\uparrow\rangle - i\sin\varphi_s|S_\uparrow\rangle = e^{-i\varphi_s}|0\uparrow\rangle - e^{i\varphi_s}|\uparrow 0\rangle , \quad (5)$$

for the generation of a "twisted-odd" doublet, and the twisted "even" vertex

$$|\widetilde{S_\uparrow}\rangle = \cos\varphi_s|S_\uparrow\rangle - i\sin\varphi_s|A_\uparrow\rangle = e^{-i\varphi_s}|0\uparrow\rangle + e^{i\varphi_s}|\uparrow 0\rangle , \quad (6)$$

for an orthogonal "twisted-even" doublet, where $\varphi_s = k_sR/2$. Thus, for the "twisted odd" doublet the w_k components of the Kondo-doublet cloud are

$$|\uparrow\uparrow, w_{k\downarrow}\rangle = (e^{i\varphi_k} + e^{-i\varphi_k})(|\uparrow\uparrow, h_{k_+\downarrow}\rangle + |\uparrow\uparrow, h_{k_-\downarrow}\rangle) , \quad (7)$$

in the resonant set, and

$$|\sigma\overline{\sigma}, w_{k\uparrow}\rangle = e^{i(\varphi_k-2\varphi_s)}|\downarrow\uparrow, h_{\overline{k}_-\uparrow}\rangle + e^{-i(\varphi_k+2\varphi_s)}|\downarrow\uparrow, h_{\overline{k}_+\uparrow}\rangle$$
$$+e^{-i(\varphi_k-2\varphi_s)}|\uparrow\downarrow, h_{\overline{k}_-\uparrow}\rangle + e^{i(\varphi_k+2\varphi_s)}|\uparrow\downarrow, h_{\overline{k}_+\uparrow}\rangle , \quad (8)$$

in the non-resonant set. In the equations above $\varphi_k = kR/2$, and $\overline{k}_\pm = \pm k + k_s$ are the k-wave vectors of the spin up holes of energy w_k. For $|\widetilde{A_\uparrow}\rangle$ the odd doublet connectivity factor for the resonant set path is recovered, given that $\langle\widetilde{A_\uparrow}|H_V^2|\widetilde{A_\uparrow}\rangle_{\uparrow\uparrow} = 1 + \cos(kR)$. Note that the effect of the twisted vertex is to remove the RSO phases from the resonant set (compare Eq.(7) with Eq.(2)); the RSO phase effects accumulate in the non-resonant set, Eq.(8).

Kondo-like interactions can not be analyzed by standard perturbative methods ([13] pag. 155, [4] pags. 53, 149). Therefore, adding over all the possible values of the hole energy, we analyze the properties of the "twisted odd" doublet by means of the following variational wave function

$$|\widetilde{D_{o\uparrow}}\rangle = |\widetilde{A_\uparrow}\rangle + \mathbf{v}\sum_{w_k} Z(w_k)(|\uparrow\uparrow, w_{k\downarrow}\rangle + |\sigma\overline{\sigma}, w_{k\uparrow}\rangle) , \quad (9)$$

where both cloud sets must be included to account for the synergy of Kondo structures. Analytical minimization [17, 22] gives the energy of the "twisted odd" doublet

$(E_o = -2E_d - \delta_o(R))$, and the variational amplitude of the configurations in its cloud ($Z(w) = 1/(\delta_o+w)$), where δ_o is the bare (no RSO coupling) odd doublet correlation energy [17]

$$\delta_o(R) = E_F \ \exp \frac{-1}{[2 \pm C_Q(\delta_o, R)] \ J_n} \ , \qquad (10)$$

where the minus sign is for the even doublet correlation energy (δ_e) and the hole coherence factor $C_Q(\delta, R)$ ($\equiv$ ($\Sigma_w \cos{(kR)} \ Z(w))/(\Sigma_w Z(w))$) is given by

$$C_Q = \frac{\cos{(u)}[\text{Ci}(u) - \text{Ci}(t)] + \sin{(u)}[\text{Si}(u) - \text{Si}(t)]}{\ln{(1 + E_F/\delta)}} \ , \qquad (11)$$

where $t = k_F R$ and $u = k_F R(1 + \delta/E_F)$, Ci (Si) is the CosIntegral (SinIntegral) function.

Therefore, as in the RKKY case, the band RSO coupling does not modify the strength of the Kondo-doublet interaction. In Fig.2 we plot δ_o, δ_e, and the RKKY energies ($\pm\Sigma_R$, with $\Sigma_R(R) = 4\ln 2 \ J_n^2 \ E_F \ [1 - (2/\pi) \ \text{Si}(2k_F R)]$ [17, 21, 23]) as function of the inter-dot distance R. Notice that the RKKY decays faster than the Kondo-doublet interaction, at $R \simeq 2\lambda_F$ the third maximum of the odd-doublet is 25 times greater than the fifth ferromagnetic maximum of the RKKY.
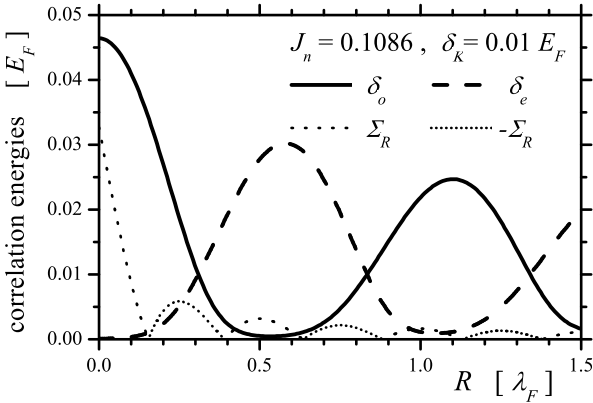

FIG. 2: Correlation energy of the Kondo-doublets and the RKKY configurations as a function of the distance between the QDs. At $R = 0$ the odd-doublet interaction is just a fifty per cent greater than the RKKY value. At $R \simeq \lambda_F$ the second maximum of the odd-doublet is already 15 times greater than the third ferromagnetic maximum of the RKKY.

But the internal structure of the doublets has been "twisted" by the RSO phase effects. These changes are reflected in the QDs spin-spin correlation. For the "twisted odd" doublet it is given by

$$\frac{\langle \widetilde{D_{o\sigma}}|S_L.S_R|\widetilde{D_{o\sigma}}\rangle}{\langle \widetilde{D_{o\sigma}}|\widetilde{D_{o\sigma}}\rangle} = \pm\frac{(1 + 2\cos 2k_s R)D_Q(R)}{4(2 \pm D_Q(R))} \ , \quad (12)$$
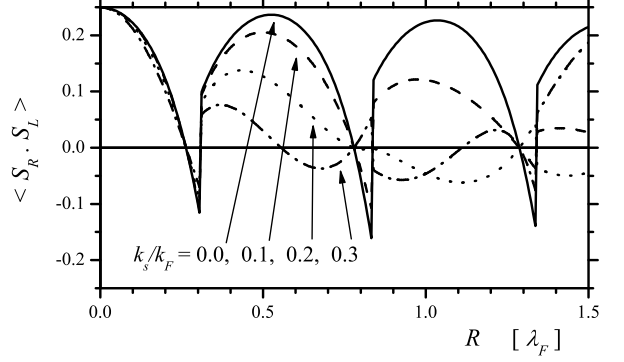

FIG. 3: QDs-spin correlation for the dominant doublet for different values of the RSO coupling. For $R \simeq \lambda_F$ a moderate value of the effective RSO coupling turns the parallel alignment of the QDs spin into a slightly antiparallel one.

where $D_Q(R) \equiv (\Sigma_w \cos{(kR)} \ Z(w)^2)/(\Sigma_w Z(w)^2)$ and the lower sign holds for the "twisted even" doublet.

In Fig.3 we plot $\langle S_L.S_R \rangle$ for the dominant doublet (i.e. that with the highest $\delta(R)$) for different values of the effective RSO coupling k_s. As the twisting angle is given by $2k_s R$ this effect is greater the greater R. This amplification property of R on the RSO effects must be balanced, in an experimental setup, with the fact that the correlation between the QDs decays due to the increasing decoherence of the hole packet that generates the Kondo-doublet interaction. A good experimental compromise is $R \simeq \lambda_F$, about a few dozen nanometers for these heterostructures. For this distance a moderate transversal electric field can turn the parallel spin alignment typical of the dominant Kondo-doublet into a slightly antiparallel one. In Fig.4 we show $\langle S_L.S_R \rangle$ for the dominant "odd" doublet at $R = 1.1\lambda_F$ as a function of the RSO coupling.
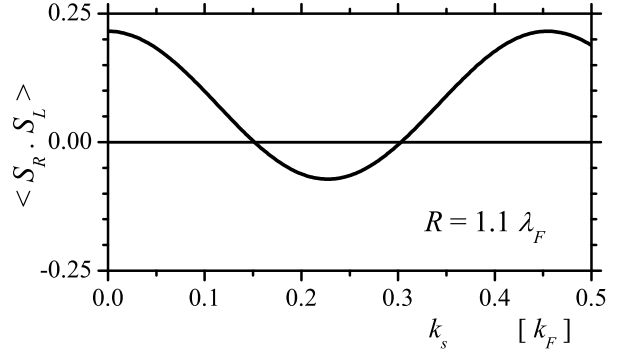

FIG. 4: QDs-spin correlation for the dominant "odd" doublet at $R = 1.1\lambda_F$ as a function of the RSO coupling.

We compare the effects of the RSO on the Kondo-

doublets with those on the RKKY. We recalculate the results of Ref.[21], which can be summarized as follows: the strength of the RKKY does not change (apart from the Fermi energy renormalization discussed previously), but the structure of the RKKY configurations is "twisted". Two of the eigenvectors of the Imamura RKKY-RSO Hamiltonian (Ref.[21], Eq.(19) plus a $-\Sigma_R/2$ term) are, in our axis setup, the $|S_z| = 1$ components of the zero-RSO ferromagnetic triplet ($|\uparrow\uparrow\rangle$ and $|\downarrow\downarrow\rangle$) with a correlation energy gain Σ_R, and the other two are a twisted mixture of the two $S_z = 0$ configurations, the odd ferromagnetic $|FM0\rangle$) and the even antiferromagnetic $|AF0\rangle$ ones $((|\downarrow\uparrow\rangle \pm |\uparrow\downarrow\rangle)/\sqrt{2})$. The twisted "ferromagnet", with a correlation energy gain Σ_R, is given by

$$
\widetilde{|FM0\rangle} = \cos 4\varphi_s |FM0\rangle + i \sin 4\varphi_s |AF0\rangle =
$$
$$
e^{i2\varphi_s}|\downarrow\uparrow\rangle + e^{-i2\varphi_s}|\uparrow\downarrow\rangle \qquad , \quad (13)
$$

and the twisted "antiferromagnet", of energy gain $-\Sigma_R$, by

$$
\widetilde{|AF0\rangle} = \cos 4\varphi_s |AF0\rangle + i \sin 4\varphi_s |FM0\rangle . \qquad (14)
$$

Direct evaluation of $\langle S_R.S_L \rangle$ for the twisted ferromagnet gives $(2\cos 2k_s R - 1)/4$. Note that the phase generated by the RSO between the $|\sigma\bar{\sigma}\rangle$ QDs configurations is the same for both the RKKY and the Kondo-doublet (Eq.(13) and Eq.(8)), resulting in the $\cos 2k_s R$ terms in their $\langle S_R.S_L \rangle$ correlations.

To distinguish between the Kondo-doublet and RKKY contributions in the experimental setup one can rely on the different dependences of their correlation energies on $k_F R$. While the RKKY depends on $2k_F R$, the Kondo-doublet depends just on $k_F R$, see Fig. 2. This is due to the fact that the fourth order RKKY path involves two band excitations, an electron and a hole, whereas the second order Kondo-doublet path involves just a hole. For the same reason the RKKY decays more quickly, as a function of R, than the Kondo-doublet. The same lateral gate voltages that generate the transversal RSO electric field can be used to modify k_F.

Conclusions. We have found that the strength of the Kondo-doublet interaction is more than an order of magnitude greater than that of the RKKY in semiconductor Kondo QD-QW systems. Therefore, to assume that the interaction between Anderson-Kondo impurities is given by the RKKY process alone, as is usually done, misses the physics of the problem. We also found that the wire Rashba spin orbit coupling can be used to control the spin correlation between QDs through the effects that it induces on the Kondo-doublet interaction. The proposed experimental setup allows also to discriminate between Kondo-doublet and RKKY contributions. Although we center the present work on the semiconductor QDs-QW data, the system can be realized also with other nano-techniques, as reported in Ref.[24].

Finally, we briefly address the implications of this work on the Kondo screening cloud pursuit [25, 26, 27]. The Kondo-doublet screening cloud is essentially the single impurity cloud [22] amplified by the resonant "pinning" of one of its components to both QDs. Thus, the measurement of the Kondo-doublet predictions is a direct test of the single impurity Kondo cloud.

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